



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2018 – 11:35 AM EST

PDB ID : 6B9M  
Title : Crystal structure of UHRF1 TTD domain in complex with the polybasic region  
Authors : Song, J.; Tan, X.  
Deposited on : 2017-10-10  
Resolution : 1.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

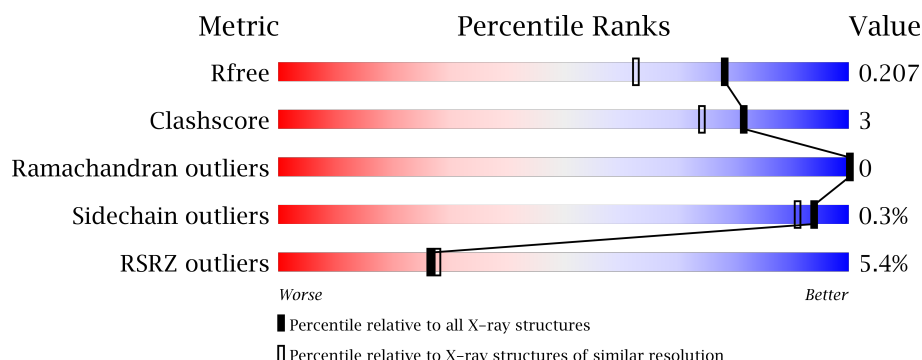
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>3%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	B	153	<div> <div>9%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	C	153	<div> <div>4%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
2	D	41	<div> <div>34%</div> <div>7%</div> <div>59%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4312 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	1	0
			1233	787	215	226	5			
1	B	148	Total	C	N	O	S	0	0	0
			1217	777	210	225	5			
1	C	150	Total	C	N	O	S	0	0	0
			1208	773	205	225	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SER	-	expression tag	UNP E7EZF3
A	171	PRO	ALA	SEE REMARK 999	UNP E7EZF3
A	173	GLU	ASP	SEE REMARK 999	UNP E7EZF3
A	207	ARG	HIS	SEE REMARK 999	UNP E7EZF3
B	128	SER	-	expression tag	UNP E7EZF3
B	171	PRO	ALA	SEE REMARK 999	UNP E7EZF3
B	173	GLU	ASP	SEE REMARK 999	UNP E7EZF3
B	207	ARG	HIS	SEE REMARK 999	UNP E7EZF3
C	128	SER	-	expression tag	UNP E7EZF3
C	171	PRO	ALA	SEE REMARK 999	UNP E7EZF3
C	173	GLU	ASP	SEE REMARK 999	UNP E7EZF3
C	207	ARG	HIS	SEE REMARK 999	UNP E7EZF3

- Molecule 2 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	0	0	0
			119	69	31	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total 179	O 179	0	0
3	B	185	Total 185	O 185	0	0
3	C	151	Total 151	O 151	0	0
3	D	20	Total 20	O 20	0	0

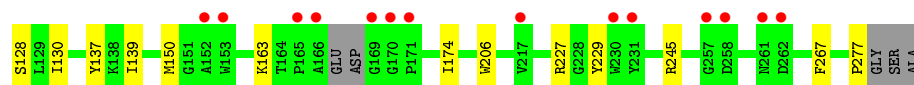
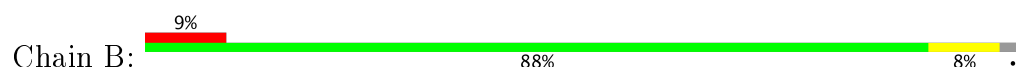
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

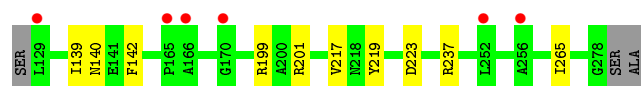
- Molecule 1: E3 ubiquitin-protein ligase UHRF1



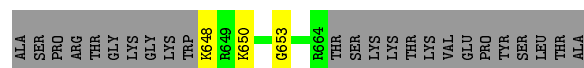
- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 2: E3 ubiquitin-protein ligase UHRF1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.22Å 66.14Å 120.58Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	28.76 – 1.68 28.76 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.76-1.68) 98.3 (28.76-1.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.182 , 0.207 0.182 , 0.207	Depositor DCC
$R_{free}$ test set	3413 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.52	0/1266	0.60	0/1712
1	B	0.46	0/1246	0.58	0/1684
1	C	0.42	0/1238	0.56	0/1678
2	D	0.53	0/120	0.78	0/155
All	All	0.47	0/3870	0.59	0/5229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1233	0	1198	5	0
1	B	1217	0	1184	9	0
1	C	1208	0	1151	6	0
2	D	119	0	128	3	0
3	A	179	0	0	2	2
3	B	185	0	0	1	2
3	C	151	0	0	3	0
3	D	20	0	0	2	0
All	All	4312	0	3661	22	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:TYR:OH	3:C:301:HOH:O	2.12	0.67
2:D:648:LYS:N	3:D:702:HOH:O	2.28	0.67
1:B:150:MET:HE1	1:B:229:TYR:HB2	1.77	0.67
1:A:273:LYS:NZ	3:A:303:HOH:O	2.33	0.61
1:C:237:ARG:HD2	3:C:314:HOH:O	2.03	0.59
1:B:130:ILE:HB	1:B:139:ILE:HB	1.87	0.56
1:C:217:VAL:HG21	1:C:265:ILE:HD12	1.87	0.56
2:D:653:GLY:O	3:D:701:HOH:O	2.18	0.56
1:B:150:MET:HE1	1:B:229:TYR:CB	2.36	0.54
1:B:137:TYR:OH	1:B:277:PRO:HG3	2.08	0.53
1:B:227:ARG:HG2	1:B:267:PHE:CZ	2.46	0.51
1:B:128:SER:N	3:B:305:HOH:O	2.44	0.49
1:A:182:ASP:OD1	3:A:302:HOH:O	2.20	0.48
1:B:206:TRP:CB	1:B:245:ARG:HH11	2.29	0.46
1:B:150:MET:CE	1:B:229:TYR:HB2	2.46	0.45
1:A:146[B]:ARG:HD2	1:A:195:ASP:OD1	2.18	0.44
1:A:227:ARG:CD	2:D:650:LYS:HG3	2.48	0.43
1:C:201:ARG:HD3	3:C:360:HOH:O	2.19	0.42
1:B:163:LYS:HG2	1:B:174:ILE:HD13	2.01	0.41
1:C:142:PHE:HB3	1:C:199:ARG:CZ	2.51	0.41
1:C:139:ILE:O	1:C:140:ASN:HB2	2.21	0.41
1:A:129:LEU:HB3	1:A:138:LYS:CB	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:458:HOH:O	3:B:400:HOH:O[3_545]	2.11	0.09
3:A:441:HOH:O	3:B:442:HOH:O[2_757]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/153 (97%)	145 (97%)	4 (3%)	0	100	100
1	B	144/153 (94%)	138 (96%)	6 (4%)	0	100	100
1	C	148/153 (97%)	146 (99%)	2 (1%)	0	100	100
2	D	15/41 (37%)	15 (100%)	0	0	100	100
All	All	456/500 (91%)	444 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/132 (97%)	128 (100%)	0	100	100
1	B	128/132 (97%)	128 (100%)	0	100	100
1	C	123/132 (93%)	122 (99%)	1 (1%)	85	76
2	D	11/31 (36%)	11 (100%)	0	100	100
All	All	390/427 (91%)	389 (100%)	1 (0%)	94	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	223	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	150/153 (98%)	-0.02	5 (3%) 47 51	22, 34, 60, 87	0
1	B	148/153 (96%)	0.51	14 (9%) 9 9	22, 42, 78, 97	0
1	C	150/153 (98%)	0.16	6 (4%) 39 42	25, 42, 77, 89	0
2	D	17/41 (41%)	-0.10	0 100 100	23, 30, 52, 57	0
All	All	465/500 (93%)	0.20	25 (5%) 26 28	22, 38, 73, 97	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ALA	8.5
1	B	170	GLY	5.8
1	B	171	PRO	5.8
1	B	169	GLY	5.8
1	A	167	GLU	4.2
1	B	152	ALA	4.2
1	A	257	GLY	4.2
1	A	256	ALA	4.0
1	B	165	PRO	3.7
1	B	258	ASP	3.5
1	C	166	ALA	3.4
1	C	165	PRO	3.1
1	C	129	LEU	3.1
1	B	231	TYR	3.0
1	B	261	ASN	2.8
1	B	257	GLY	2.8
1	C	252	LEU	2.7
1	B	262	ASP	2.6
1	A	258	ASP	2.6
1	B	230	TRP	2.5
1	B	217	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	256	ALA	2.3
1	B	153	TRP	2.1
1	C	170	GLY	2.1
1	A	128	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.